

CHEMICAL TRACKING

Purpose This Meteorology and Air Quality Group (MAQ) procedure describes the process for reviewing and evaluating chemical procurement records as a method of identifying and quantifying regulated chemicals.

Scope This procedure applies, when referred from another procedure, to the identification and quantification of regulated chemicals purchased and used at LANL, including Hazardous Air Pollutants (HAPs); Volatile Organic Compounds (VOCs); 112r Chemicals; SARA 313 Toxic Chemicals; and Toxic Air Pollutants (TAPs). This procedure is not intended to describe the requirements or to instruct on compliance with the various rules and regulations.

In this procedure This procedure addresses the following major topics:

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General Information about this Procedure

Attachments This procedure has the following attachments:

Number	Attachment Title	Pages
1	Flow chart	1

History of revision This table lists the revision history and effective dates of this procedure.

Revision	Date	Description Of Changes
0	1/20/98	New document.
1		Revised to reflect new chemical tracking system.

Who requires training to this procedure? The following personnel require training before implementing this procedure:

- individuals assigned to track (for air quality compliance reporting) regulated chemicals procured and used at LANL

Training method The training method for this procedure is **on-the-job** training by a previously-trained individual and is documented in accordance with the procedure for training (MAQ-024).

Prerequisites Individuals training to this procedure need to have experience with Microsoft Access and ChemLog, the Laboratory's chemical tracking database.

Definitions specific to this procedure

CAS numbers: Chemical Abstracts Service number that identifies chemicals.

HAPs: Hazardous Air Pollutants [defined by CAA (b)]

TAPs: Toxic Air Pollutants [defined by NMAQ 2.72.502]

References The following documents are referenced in this procedure:

- MAQ-024, "Personnel Training"
- MAQ-310, "EPCRA 313 Reporting"
- MAQ-317, "Emissions Reporting"
- MAQ-327, "Threshold Determinations for CAA Section 112r"

Obtaining Chemical Procurement Data

Primary source of data

ChemLog is a database containing Laboratory-wide procurement and inventory records for chemicals. It is the most comprehensive source of procurement records and is a good starting point for the identification of regulated chemicals purchased by LANL. HSR-5 personnel can help to identify any deficiencies found in the data and may suggest methods, resources, or provide additional data to correct deficiencies.

Overcoming data gaps

Supplemental data should be used when they are available and when ChemLog deficiencies are identified.

Pull data together from additional sources, including but not limited to:

- project managers (primarily large purchases)
 - orders tracked by SUP Division (primarily large purchases)
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How the pounds text file is automatically created

The following automated steps import ChemLog data daily to a text document called “ex3_daily_lb.txt” located at `cleanair.lanl.gov:USERS\FTPPFILES\DAILY`.

- Data from the ChemLog tables, located at `safety.lanl.gov`, is loaded into a file called `ex3_daily.txt`.
- For each record, the CAS number, the physical state, the unit of measure (UOM), and the container size from the ChemLog tables are checked for data accuracy against two text tables. The text tables are called “units.txt” and “gasplant.txt” and are located at `/export/home/u094014` on `safety.lanl.gov`. If there is a discrepancy, the pounds calculation is performed twice, once with the errored value and once with a substituted value.
- Physical properties along with UOM and container size are necessary to calculate pounds of a chemical. Properties are stored in UNIX dbm files `chemtox.pag` and `mdl.pag` at `/static/export/home/u094014`.
- A mass conversion calculation for each record is then performed by the following criteria:
 - for liquids, the chemical’s specific gravity is used,
 - for gases, the ideal gas law at standard temperature (20° C) and standard pressure (1 atm) is used, and
 - for solids, simple conversion of units (kilograms, ounces, tons, etc.) to pounds is used.
- If the information to convert the quantity to pounds is not available, the following default values are used: for liquids the specific gravity of water (1) and for gases the molecular weight of air (28.9 g/mole).
- Finally, the record is written to the “ex3_daily_lb.txt” file.

Obtaining Chemical Procurement Data, continued

Contents of text file

The text file includes, but is not limited to the following ChemLog fields:

- barcode
- chemical name
- CAS number
- manufacturer
- catalog number
- order number
- physical state
- container size
- unit of measure
- container add date
- technical area
- building number
- purchaser's name
- group name.

Additionally, the text file will also include a calculated field called "MAQ_lb" which is a conversion of all quantities to pounds.

Regulated chemical lists

List of regulated chemicals by CAS number can be found on the Projects drive. The lists of regulated chemicals may change periodically. Ensure that the most up-to-date lists are used for this evaluation. These lists can be located in EPA documents, on the regulatory agencies' Internet web pages, or from other reliable resources. These lists may include HAPs, VOCs, 112r, SARA 313, TAPs or other regulated chemical lists.

Processing and Evaluating Chemical Data

Compile electronic files

Import the text document “ex3_daily_lb.txt” (obtained as described in the previous chapter) into an Access database. These files should include the chemical data. Also, import the regulated chemical list from the previous year’s database located on the Projects drive at \\Emission Inventory for Emissions Inventory chemicals and on the Projects drive at \\EPCRA for EPCRA 313 chemicals. Supporting files may include composition information, concentration, and specific gravities listed by CAS numbers. If available, use commercial files for the composition information and specific gravities. Otherwise, use best available data (e.g., MSDSs or other chemical references).

Review data for errors

MAQ has also developed an automated tool to convert purchasing records to pounds. The MAQ conversion makes use of more detailed physical property information. The “MAQ_lb” and the “ex3_lb” fields should be compared as a QA check on the conversion process. Discrepancies should be identified and investigated to determine which is correct.

To review data for data entry errors, perform the following steps:

Step	Action
1	Select the chemical data for the date range to be analyzed.
2	Check the number of records and compare to the previous years download.
3	Rank the totals of each chemical by quantity.
4	Start with the chemicals with the largest totals. Call the purchasers of quantities that seem abnormally high to determine actual quantity and chemical purchased. Make all corrections in database.
5	Analyze purchases with quantities of zero. Call the purchasers of the chemicals to determine actual quantity and chemical purchased. Make all corrections in database.
6	Review dates for any gaps in the data. If any are found, contact HSR-5 for an explanation.

Processing and Evaluating Chemical Data, continued

Refine the data

After the above steps, the chemical data of interest have been refined from a large amount of data. The data can be further refined to meet the specific reporting requirements of the applicable rule or regulation.

Document the work

Document the process assumptions that were used when this procedure was followed. Document any steps that were not followed or other deviations from the specified process. The level of documentation should be sufficient to demonstrate compliance with the applicable regulation and to allow duplication of the process.

Records Resulting from this Procedure

Records

The following records are to be submitted **as specified in the referring procedure** (MAQ 310, “EPCRA 313 Reporting”; MAQ 317, “Emissions Reporting”; MAQ 327, “Threshold Determinations for CAA Section 112r”) as records to the records coordinator:

- chemical data results of the evaluation
- assumptions made in the evaluation
- limitations of the data
- annotated process description and list of deviations and assumptions, as appropriate, that will allow duplication of the process

FLOW CHART OF CHEMICAL TRACKING PROCESS

